Method 2: Bernstein's inequality for matrices

Theorem

(Tropp'15) Let X_1, \ldots, X_m be independent Hermitian random matrices such that: $\mathbb{E}(X_k) = 0$, $||X_k||_{op} \leq L$ almost surely, $k \in [m]$.

Let $Y = \sum_{k \in [m]} X_k$, and $v(Y) := \|\mathbb{E}(Y^2)\|_{op} = \|\sum_{k \in [m]} \mathbb{E}X_k^2\|_{op}$. Then for all t > 0, $\mathbb{P}(\lambda_1(Y) \ge t) \le n \exp\left(\frac{-t^2}{2(v(Y)+Lt/3)}\right)$. This implies for all t > 0: $\mathbb{P}(\|Y\|_{op} \ge t) \le 2n \exp\left(\frac{-t^2}{2(v(Y)+Lt/3)}\right)$.

Corollary

For W s.t. W_{ij} independent up to symmetry, $\mathbb{E}W_{ij} = 0$, $|W_{ij}| \le 1$, $\mathbb{E}W_{ij}^2 = O(d/n)$: If $d \gg \log(n)$ then with high probability $\rho(W) = o(d)$.

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Stronger bounds on $\rho = \rho(W)$

Theorem (Feige and Ofek, 2005)

Let $A \in \mathbb{R}^{n \times n}$: symmetric matrix with entries independent up to symmetry, $A_{ij} \in [0,1]$, and such that $\mathbb{E}(A_{ij}) \leq d/n$, where $d \leq n^{1/5}$. Then for some (universal) constant $\kappa > 0$, with high probability $\rho(A - \mathbb{E}(A)) \leq \kappa \sqrt{\max(d, \log(n))}$.

Corollary

For $d \gg \sqrt{\max(d, \log(n))}$, i.e. $d \gg \sqrt{\log(n)}$, with high probability $\rho(A - \mathbb{E}A) = o(d)$

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Proof of Bernstein matrix inequality

Lemma

For independent Hermitian matrices X_k , $k \in [m]$, and $Y = \sum_{k \in [m]} X_k$:

$$\mathbb{E}\mathrm{Tr}e^{\theta Y} \leq \mathrm{Tr}\exp\left(\sum_{k\in[m]}\ln\mathbb{E}e^{\theta X_k}\right)$$

Lemma

For Hermitian X such that $\mathbb{E}(X) = 0$ and $||X|| \le L$ almost surely, then:

$$orall heta \in (0, 3/L), \ \left\{ egin{array}{ll} \mathbb{E} e^{ heta X} \preceq \exp\left(rac{ heta^{2}/2}{1- heta L/3}\mathbb{E}X^{2}
ight), \ \ln \mathbb{E} e^{ heta X} \preceq rac{ heta^{2}/2}{1- heta L/3}\mathbb{E}X^{2}, \end{array}
ight.$$

Lemma

For Hermitian A, B, if $A \leq B$, then $\forall i \in [n], \lambda_i(A) \leq \lambda_i(B)$. Hence for all non-decreasing $f : \mathbb{R} \to \mathbb{R}$, $\operatorname{Tr} f(A) \leq \operatorname{Tr} f(B)$.

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Application: Community Detection in the Stochastic Block Model

 $\mathcal{G}(n, \{\alpha_i\}_{i \in [K]}, P)$, where $\alpha_i > 0, \sum_{i \in [K]} \alpha_i = 1, P \in [0, 1]^{K \times K}$: multi-type version of the Erdős-Rényi random graph

- *n* vertices partitioned into *K* communities
- Type (community) of node $i : \sigma_i \in [K], \sigma_i : i.i.d., \sim \alpha$
- Conditionally on σ_[n], independently for each pair i, j ∈ [n]: edge (i, j) present with probability P_{σ(i),σ(j)}.

Strong signal regime: fixed $K, \alpha, B \in \mathbb{R}^{K \times K}_+$; P = (d/n)B, with $\lim_{n \to +\infty} d = +\infty$

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Spectral embedding

- Extract top two (more generally top *R*) eigenvalues λ_1, λ_2 of graph's adjacency matrix $A \in \mathbb{R}^{n \times n}$ (ordered by absolute value: $|\lambda_1| \ge |\lambda_2| \ge \cdots$)
- Let $x_1, x_2 \in \mathbb{R}^n$: corresponding normalized eigenvectors
- Embed vertex $k \in [n]$ into \mathbb{R}^2 by letting $z_k := \sqrt{n}(x_1(k), x_2(k))$

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- Embed vertex $k \in [n]$ into \mathbb{R}^2 by letting $z_k := \sqrt{n}(x_1(k), x_2(k))$
- \rightarrow based on PCA dimensionality reduction of A to dimension R

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Example: spectral embedding for SBM



A case with K = 4 communities Spectral embedding seems to reflect community structure \rightarrow Why / when do spectral methods work?

Theorem

Assume communities are **distinguishable**, *i.e.* for each $k \neq l \in [K]$, there exists $m \in [K]$ such that $B_{km} \neq B_{\ell m}$.

Assume $\sqrt{\ln(n)} \ll d \ll n^{\delta}$ for some fixed $\delta \in]0,1[$. Let *R*: rank of matrix *B*. Then with high probability:

(i) the spectrum of A consists of R eigenvalues of order $\Theta(d)$ and n - R eigenvalues of order o(d).

(ii) *R*-dimensional spectral embedding reveals underlying communities: except for vanishing fraction of nodes $i \in [n]$,

$$||z_i - z_j|| = \begin{cases} o(1) & \text{if } \sigma(i) = \sigma(j), \\ \Omega(1) & \text{if } \sigma(i) \neq \sigma(j) \end{cases}$$

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Corollary

Under these conditions any sensible clustering scheme (eg K-means properly initialized) correctly classifies all but vanishing fraction of nodes.

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Proof strategy



- \bar{A} : block matrix (useful "signal")
- Write adjacency matrix as $A = \overline{A} + W$ with $\overline{A}_{ij} = \frac{d}{n} B_{\sigma(i),\sigma(j)}$
- R leading eigen-elements of \overline{A} capture community structure
- Control perturbation of eigen-elements of a symmetric matrix A by addition of symmetric matrix W in terms of spectral radius ρ(W) of noise matrix
- Prove bound on $\rho(W)$ for random noise matrix W

Eigenstructure of \overline{A}

Block structure of $\overline{A} \Rightarrow \overline{A}x$ constant on each block \Rightarrow eigenvectors associated to non-zero eigenvalue are block-constant.

For $t \in \mathbb{R}^{K}$ define $x := \phi(t) = (t_{\sigma(i)})_{i \in [n]} \in \mathbb{R}^{n}$.

Then $\overline{A}\phi(t) = d\phi(Mt)$, where $M_{uv} := B_{uv}\alpha_v$.

Lemma

Spectrum of \overline{A} : R eigen-pairs ($\lambda_u = d\mu_u, \overline{x}_u = \phi(t_u)$) where (μ_u, t_u): eigen-pairs of Mwith $\mu_u \neq 0$; 0: eigenvalue with multiplicity n - R

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Eigenstructure of \overline{A} (continued)

Lemma

Under distinguishability hypothesis there exists $\epsilon > 0$ function of B, α such that for any choice of normalized leading eigenvectors $\overline{x}_1, \ldots, \overline{x}_R$, $\overline{z}_i = \sqrt{n}(\overline{x}_1(i), \ldots, \overline{x}_R(i))^T$ verify

 $\sigma(i) \neq \sigma(j) \Rightarrow \|\overline{z}_i - \overline{z}_j\| \ge \epsilon > 0$

Proof: Let $t_u \in \mathbb{R}^K$ be such that $\sqrt{n\overline{x}_u} = \phi(t_u)$, and $\sqrt{\alpha} = \text{Diag}(\sqrt{\alpha_u})$. Then: $\{\sqrt{\alpha}t_u\}_{u\in[R]}$: orthonormal family by orthonormality of the \overline{x}_u . t_u eigenvectors of matrix $M = B\alpha$, hence $\sqrt{\alpha}t_u$: orthonormal family of eigenvectors of matrix $\sqrt{\alpha}B\sqrt{\alpha}$. Thus $\sqrt{\alpha}B\sqrt{\alpha} = \sum_{u\in[R]} \mu_u(\sqrt{\alpha}t_u)(\sqrt{\alpha}t_u)^T$. Equivalently: $B = \sum_{u\in[R]} \mu_u t_u t_u^T$. Hence minimum of $\|\overline{z}_i - \overline{z}_j\|$ over $\sigma(i) \neq \sigma(j)$ strictly positive, for otherwise *B* has two identical rows, i.e. distinguishability fails.

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Proof

- Matrix A of rank R, spectral gaps |λ_i λ_j| = Ω(d), R-dimensional spectral embedding with x₁,..., x_R separates clusters V_k = {i ∈ [n] : σ_i = k}
- Feige-Ofek: d ≫ √log n ⇒ ρ := ρ(A Ā) ≪ d. Weyl's inequality: R eigenvalues λ_i close to λ_i = Θ(d), others of order ρ ≪ d
- Davis-Kahane: eigenvectors x_i such that $\langle x_i, \overline{x}_i \rangle = 1 O((\rho/d)^2)$

Then $\sum_{i \in [n]} ||z_i - \overline{z}_i||^2 = n \sum_{u \in [R]} ||x_u - \overline{x}_u||^2 = n\theta$ with $\theta = O((\rho/d)^2) = o(1)$ Hence (Tchebitchev inequality): $|\{i : ||z_i - \overline{z}_i|| \ge \theta^{1/3}\}| < n\theta^{1/3} = o(n)$

Yields desired conclusion: except for vanishing fraction $\theta^{1/3}$ of nodes, spectral representatives $z_i \ \theta^{1/3}$ -close of corresponding \overline{z}_i , themselves clustered according to community structure

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Graphon model

Let \mathcal{X} : compact metric space, π : probability measure on \mathcal{X} , $P(x, y) : \mathcal{X}^2 \to [0, 1]$: continuous symmetric function

Definition

Graphon $\mathcal{G}(n, \pi, P)$: σ_i i.i.d. $\sim \pi$. Conditionally on $\sigma_{[n]}$, $(A_{i,j})_{i < j}$: independent, $\sim \text{Ber}(P(\sigma_i, \sigma_j))$.

Focus on strong signal regime: Graphon $\mathcal{G}(n, \pi, (d/n)K)$ for fixed π and kernel K, and signal strength $d \to \infty$

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Operator theory background

Theorem

(Kato'66) Let T: linear self-adjoint operator on Hilbert space $\mathbb{L}^2(\pi)$ where π : non-negative measure be **compact**, i.e. for any bounded set C, $\overline{T(C)}$ is compact.

Then: T admits discrete real spectrum $\{\lambda_k\}_{k\geq 1}$ and associated orthonormal collection of eigenfunctions $\{\psi_k\}_{k\geq 1}$ such that $Tf(x) = \sum_{k\geq 1} \lambda_k \psi_k(x) \int_{\mathcal{X}} \psi_k(y) f(y) \pi(dy).$

Special case: for compact \mathcal{X} , continuous symmetric kernel $K : \mathcal{X}^2 \to \mathbb{R}$, associated operator $T : Tf(x) = \int_{\mathcal{X}} K(x, y)f(y)\pi(dy)$ is compact. Its eigen-elements $\{\lambda_k\}_{k\geq 1}, \{\psi_k\}_{k\geq 1}$ verify $K(x, y) = \sum_{k\geq 1} \lambda_k \psi_k(x)\psi_k(y),$ $\sum_{k\geq 1} \lambda_k^2 = \int_{\mathcal{X}^2} K(x, y)^2 \pi(dx)\pi(dy).$

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Koltchinskii-Giné Theorem

Theorem

For compact \mathcal{X} endowed with probability measure π , continuous symmetric kernel $K: \mathcal{X}^2 \to \mathbb{R}$, associated operator T, positive part of its spectrum $\{\lambda_i^+\}_{i\geq 1}$: $\lambda_1^+ \geq \lambda_2^+ \geq \cdots \geq 0$. Let $\{\sigma_i\}_{i\geq 1}$: *i.i.d.*, $\sim \pi$, and $M = \frac{1}{n} (K(\sigma_i, \sigma_j))_{i,i\in[n]}$. Let $i_0: \lambda_{i_0-1}^+ > \lambda_{i_0}^+ = \dots = \lambda_{i_0+d-1}^+ > \lambda_{i_0+d}^+$. (*d*-dimensional eigenspace) Let $\lambda_i^{+,n}$: positive eigenvalues of M, and associated ON eigenvectors $v_i^{+,n}$. Then for $i = i_0, ..., i_0 + d - 1$: $\lambda_i^{+,n} \to \lambda_i^+$ in probability as $n \to \infty$; There exist orthonormal eigenfunctions ψ_i^+ of **T** such that $\left\|v_{j}^{+,n}-\frac{1}{\sqrt{n}}\{\psi_{j}(\sigma_{k})\}_{k\in[n]}\right\|\to 0$ in probability as $n\to\infty$.

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Graphon reconstruction, strong signal regime

Theorem

Let $A \sim \mathcal{G}(n, \pi, (d/n)K)$. Let $R \geq 1$ be fixed such that $|\lambda_{R+1}(T)| < |\lambda_R(T)|$. Let u_1, \ldots, u_R : orthonormal collection of eigenvectors of A associated with $\lambda_1(A), \ldots, \lambda_R(A)$. Assume that $\sqrt{\log n} \ll d \ll n^{\delta}$ for some fixed $\delta \in (0, 1)$. Define

$$\hat{\mathcal{K}}_{ij} = \sum_{\ell=1}^{R} \lambda_{\ell}(\mathcal{A}) u_{\ell}(i) u_{\ell}(j), \ i, j \in [n].$$

Then with high probability

$$\sum_{i,j\in[n]} \left[\frac{n}{d} \hat{K}_{ij} - \mathcal{K}(\sigma_i,\sigma_j) \right]^2 = o(n^2) + O(n^2 \epsilon_R^2),$$

where $\sigma_i \in \mathcal{X}$: type of vertex $i \in [n]$, and

$$\epsilon_R^2 = \sum_{\ell > R} \lambda_\ell(K)^2.$$

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Interpretation: For fraction 1 - o(1) of pairs *i*, *j*, $\hat{K}_{ij} = \frac{d}{n} K(\sigma_i, \sigma_j) [o(1) + O(\epsilon_R)].$

Proof idea: Write $A = \frac{d}{n} (K(\sigma_i, \sigma_j))_{i,j \in [n]} + W$

Feige-Ofek or Bernstein inequality: w.h.p. $\rho(W) = o(d)$.

Koltchinskii-Giné's theorem: eigen-elements of $\frac{d}{n} (K(\sigma_i, \sigma_j)) \approx d\lambda_{\ell}(T), \{ n^{-1/2} \psi_{\ell}(\sigma_k) \}_{k \in [n]}$

Hence $\hat{K}_{ij} \approx \frac{d}{n} \sum_{\ell \in [R]} \lambda_{\ell}(T) \psi_{\ell}(\sigma_i) \psi_{\ell}(\sigma_j)$. Finally $K'(x, y) := K(x, y) - \sum_{\ell \in [R]} \lambda_{\ell}(T) \psi_{\ell}(x) \psi_{\ell}(y)$ verifies LLN:

 $\frac{1}{n^2}\sum_{i,j\in[n]}[K'(\sigma_i,\sigma_j)]^2 \to \sum_{\ell>R}\lambda_\ell(T)^2 = \epsilon_R^2$

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Example

Take $\mathcal{X} = [0, 1]$, $\pi = \mathcal{U}([0, 1])$, $g : \mathbb{R} \to \mathbb{R}$ 1-periodic continuous function, and $\mathcal{K}(x, y) = g(x - y)$.

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Then spectrum of K determined by Fourier coefficients of g

Ex: for $g(x) = |x|, \ |x| \le 1/2$: $g(x) = \frac{1}{4} + \sum_{k \ge 1} \frac{(-1)^k - 1}{\pi^2 k^2} \cos(2\pi x)$

$$\lambda_1 = \frac{1}{4}, \ \lambda_{2k} = \lambda_{2k+1} = \frac{-1}{\pi^2(2k-1)^2}, \ k \ge 1.$$

 \rightarrow Power-law decay of spectrum of A

Pairwise graphical models and Markov random fields

Definition

For undirected graph $\mathcal{G} := (\mathcal{V}, \mathcal{E})$, finite alphabet \mathcal{X} , functions $\psi_i : \mathcal{X} \to \mathbb{R}_+, i \in \mathcal{V}, \psi_e : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+, e \in \mathcal{E}$, the probability distribution μ on $\mathcal{X}^{\mathcal{V}}$ defined by $\mu(x) := \frac{1}{Z} \prod_{i \in \mathcal{V}} \psi_i(x_i) \prod_{e=(i,j) \in \mathcal{E}} \psi_{i,j}(x_i, x_j)$

is a pairwise graphical model with underlying graph ${\boldsymbol{\mathcal{G}}}$

The normalization constant
$$Z = \sum_{x \in \mathcal{X}^{\mathcal{V}}} \prod_{i \in \mathcal{V}} \psi_i(x_i) \prod_{e=(i,j) \in \mathcal{E}} \psi_{i,j}(x_i, x_j)$$
 is

known as its partition function.

Example

lsing model: $\mathcal{X} = \{-1, 1\}, \psi_i(x_i) = e^{h_i x_i}, \psi_{ij}(x_i, x_j) = e^{J_{ij} x_i x_j}.$ X_i : spin at site *i*; h_i : external field at *i*; J_{ij} : coupling coefficient between sites *i* and *j*

Definition

For undirected graph $\mathcal{G} := (\mathcal{V}, \mathcal{E})$, finite alphabet \mathcal{X} , probability measure μ on $\mathcal{X}^{\mathcal{V}}$, (\mathcal{G}, μ) : Markov field if there exist functions $\psi_K : \mathcal{X}^K \to \mathbb{R}_+$ indexed by **cliques** K of \mathcal{G} and Z such that $\mu(x) = \frac{1}{Z} \prod_K \psi_K(x_K), x \in \mathcal{X}^{\mathcal{V}}$, where $x_K := (x_i)_{i \in K}$.

Easy property: For any pairwise graphical model μ with underlying graph \mathcal{G} , (μ, \mathcal{G}) is a Markov random field.

Definition

For subsets $A, B, C \subset \mathcal{V}$, C separates A and B in \mathcal{G} if any path in \mathcal{G} from A to B traverses C. We denote this $A \stackrel{C}{\underset{\mathcal{G}}{\longrightarrow}} B$.

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Hammersley-Clifford Theorem

Theorem

For Markov field (μ, \mathcal{G}) , and A, B, C such that $A - \frac{c}{\mathcal{G}} B$, then under μ , X_A and X_B are independent conditionally on X_C .

Conversely, for any probability measure μ on $\mathcal{X}^{\mathcal{V}}$ such that $\forall x \in \mathcal{X}^{\mathcal{V}}, \ \mu(x) > 0$ and for all A, B, C such that $A \stackrel{C}{\underset{\mathcal{G}}{\longrightarrow}} B$, under μ, X_A and X_B are independent conditionally on X_C , then (μ, \mathcal{G}) is a Markov field. Proof (Markov field \Rightarrow conditional independence) Let $A \stackrel{C}{\xrightarrow{g}} B$. Denote \overline{A} , resp. \overline{B} : nodes reachable from A, resp. Bwithout entering C. Let $A' = \overline{A} \setminus A$, $B' = \overline{B} \setminus B$.

Lemma

 \overline{A} and \overline{B} are disjoint. Any clique K of \mathcal{G} is included in $\overline{A} \cup C$ or in $\overline{B} \cup C$.

Corollary

For Markov field (μ, \mathcal{G}) there exist functions F, G such that for any $x \in \mathcal{X}^{\mathcal{V}}, \ \mu(x) = F(x_{\overline{A} \cup C})G(x_{\overline{B} \cup C}).$

Thus: $\mathbb{P}(X_{A\cup C} = x_{A\cup C}) = \sum_{y_{A'}, y_{\bar{B}}} F(x_{A\cup C}, y_{A'})G(y_{\bar{B}}, x_{C}),$ $\mathbb{P}(X_{B\cup C} = x_{B\cup C}) = \sum_{z_{B'}, z_{\bar{A}}} F(z_{\bar{A}}, x_{C})G(x_{B\cup C}, z_{B'}),$ $\mathbb{P}(X_{A\cup B\cup C} = x_{A\cup B\cup C}) = \sum_{y_{A'}, z_{B'}} F(x_{A\cup C}, y_{A'})G(x_{B\cup C}, z_{B'}),$ $\mathbb{P}(X_{C} = x_{C}) = \sum_{z_{\bar{A}}, y_{\bar{B}}} F(z_{\bar{A}}, x_{C})G(y_{\bar{B}}, x_{C}).$ $\Rightarrow \mathbb{P}(X_{A\cup C} = x_{A\cup C})\mathbb{P}(X_{B\cup C} = x_{B\cup C}) = \mathbb{P}(X_{A\cup B\cup C} = x_{A\cup B\cup C})\mathbb{P}(X_{C} = x_{C})$

Proof (Conditional independence \Rightarrow Markov field)

Fix $x^* \in \mathcal{X}^{\mathcal{V}}$; for $S \subset \mathcal{V}$, note $\phi_S(x_S) := \prod_{U \subseteq S} \mu(x_U, x^*_{V \setminus U})^{(-1)^{|S \setminus U|}}$

Lemma

One has $\mu(x) = \mu(x^*) \prod_{S \subseteq V, S \neq \emptyset} \phi_S(x_S)$.

Proof:

 $\prod_{S \subseteq V, S \neq \emptyset} \phi_{S}(x_{S}) = \prod_{S \subseteq V, S \neq \emptyset} \prod_{U \subset S} \mu(x_{U}, x_{\mathcal{V} \setminus U}^{*})^{(-1)^{|S \setminus U|}} = \prod_{U \subseteq \mathcal{V}} \mu(x_{U}, x_{\mathcal{V} \setminus U}^{*})^{\kappa_{U}},$ where $\kappa_{U} = \sum_{S \neq \emptyset, U \subseteq S \subseteq \mathcal{V}} (-1)^{|S \setminus U|}.$

Use
$$\sum_{B\subseteq A} (-1)^{|B|} = \sum_{B\subseteq A} (-1)^{|A\setminus B|} = \mathbb{I}_{A=\emptyset} \Rightarrow \sum_{S\subseteq \mathcal{V}} (-1)^{|S|} = 0$$
 to establish:
 $\kappa_{\emptyset} = -1, \ \kappa_{\mathcal{V}} = 1, \ \emptyset \neq U \subsetneq \mathcal{V} \Rightarrow \kappa_{U} = 0.$

Lemma

For S not a clique of \mathcal{G} , $\phi_X(x_S) \equiv 1$.

Proof: If
$$\exists j \in S : x_j = x_j^*$$
, then
 $\phi_S(x_S) = \prod_{U \subseteq S-j} \left(\frac{\mu(x_U, x_{\mathcal{V} \setminus U}^*)}{\mu(x_{U+j}, x_{\mathcal{V} \setminus (U+j)}^*)} \right)^{(-1)^{|S \setminus U|}} = 1.$
 S not a clique $\Rightarrow \exists i, j \in S : (i, j) \notin \mathcal{E}.$
 $\phi_S(x_S) = \prod_{U \subseteq S-i} \left(\frac{\mu(x_U, x_{\mathcal{V} \setminus U}^*)}{\mu(x_{U+i}, x_{\mathcal{V} \setminus (U+i)}^*)} \right)^{(-1)^{|S \setminus U|}}.$
For fixed $U \subseteq S - i, K := \mathcal{V} \setminus \{i, j\}$, let $y_k = \begin{cases} x_k & \text{if } k \in U, \\ x_k^* & \text{if } k \in \mathcal{V} \setminus U. \end{cases}$
Then, since $\{i\} - \frac{\kappa}{g} \{j\}, \frac{\mu(x_U, x_{\mathcal{V} \setminus U}^*)}{\mu(x_{U+i}, x_{\mathcal{V} \setminus (U+i)}^*)} = \frac{\mathbb{P}(X_i = x_i^* | X_K = y_K) \mathbb{P}(X_j = y_j | X_K = y_K)}{\mathbb{P}(X_i = x_i | X_K = y_K)},$ which does not depend on value $x_j.$

Thus $\phi_S(x_S) = \phi_S(x_{S-j}, x_j^*) = 1.$

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